



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:41 am GMT

PDB ID : 4CAR  
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with 7-((3-Fluorophenethylamino)methyl)quinolin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2013-10-08  
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

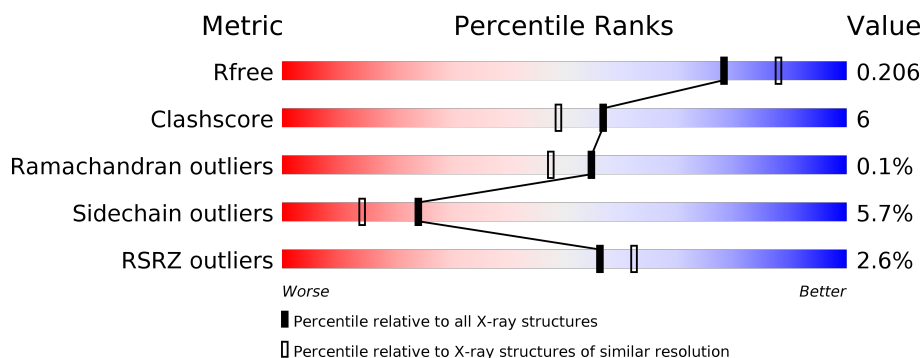
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>••</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	860	-	-	-	X
5	ACT	B	861	-	-	-	X
6	GOL	B	880	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	VARIANT	UNP P29473
B	100	ARG	CYS	VARIANT	UNP P29473

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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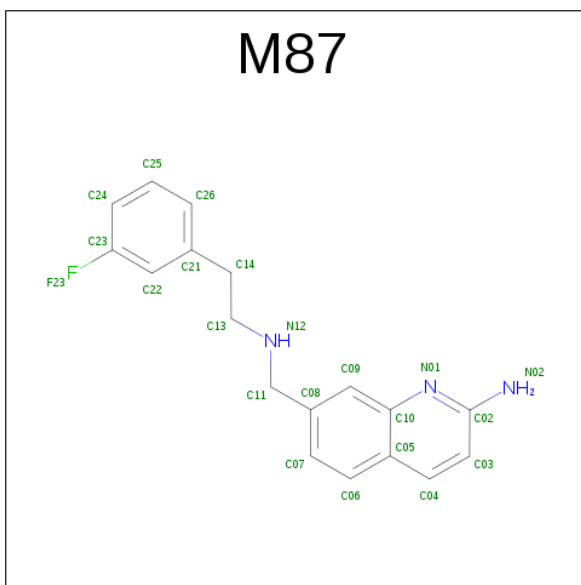
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



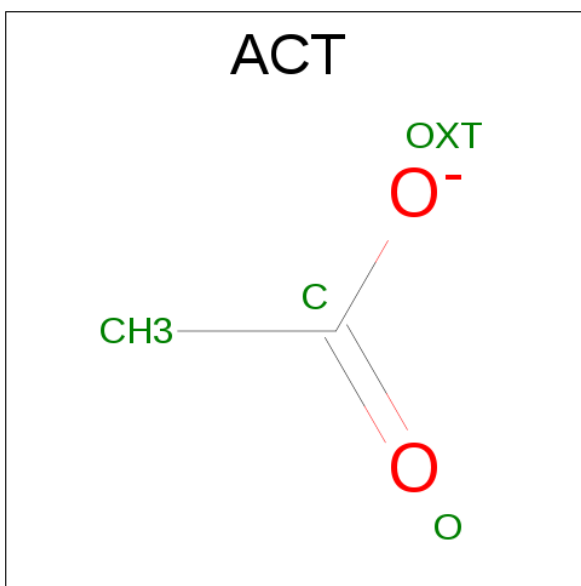
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-[[2-(3-FLUOROPHENYL)ETHYLAMINO]METHYL]QUINOLIN-2-AMINE (three-letter code: M87) (formula:  $C_{18}H_{18}FN_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			22	18	1	3		
4	B	1	Total	C	F	N	0	0
			22	18	1	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

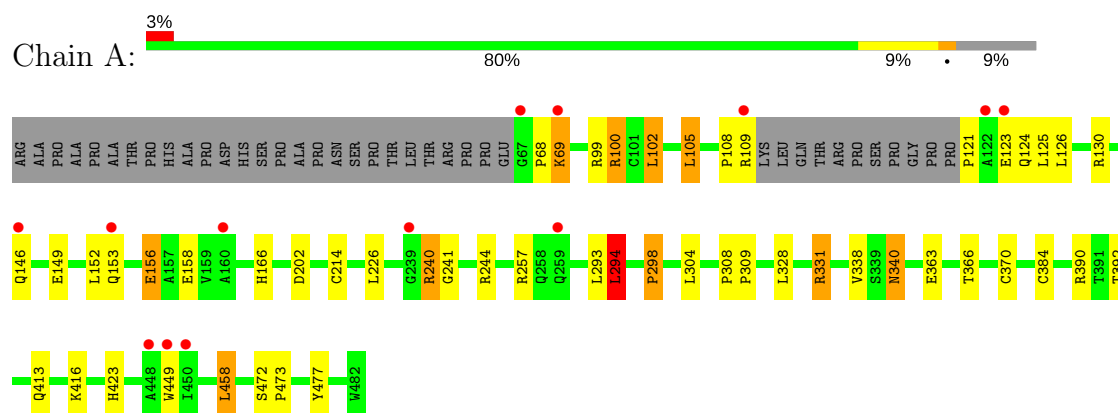
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	211	Total	O	0	0
			211	211		
8	B	175	Total	O	0	0
			175	175		

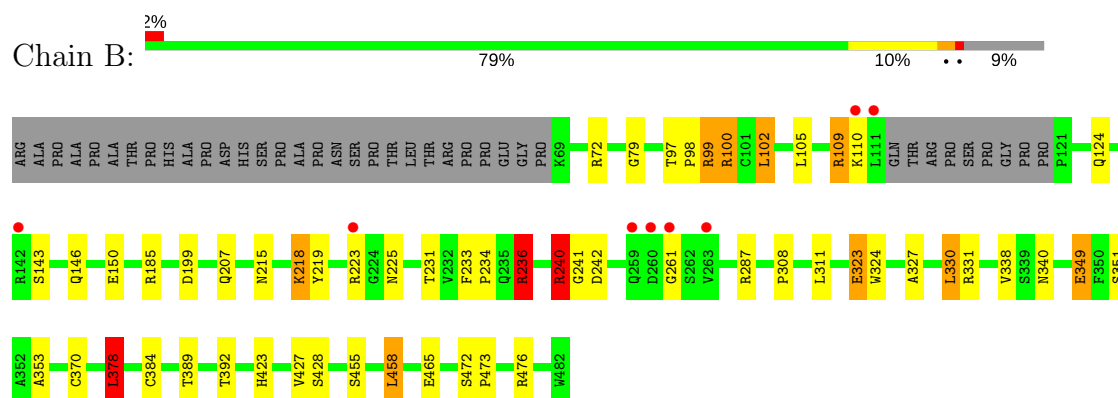
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



#### • Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.76Å 106.30Å 156.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.05 48.28 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.33-2.05) 98.5 (48.28-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.154 , 0.198 0.165 , 0.206	Depositor DCC
$R_{free}$ test set	3010 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CAS, M87, ACT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.99	0/3303	1.01	8/4497 (0.2%)
1	B	0.97	3/3308 (0.1%)	1.00	12/4502 (0.3%)
All	All	0.98	3/6611 (0.0%)	1.01	20/8999 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	GLY	C-O	-5.87	1.14	1.23
1	B	349	GLU	CD-OE2	-5.62	1.19	1.25
1	B	428	SER	CB-OG	5.37	1.49	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	B	240	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	240	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	240	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	B	185	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	331	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	100	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	378	LEU	CB-CG-CD1	6.40	121.89	111.00
1	A	331	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	330	LEU	CB-CG-CD1	6.00	121.21	111.00
1	A	244	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	72	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	294	LEU	CB-CG-CD1	5.73	120.74	111.00
1	B	242	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	199	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	458	LEU	CB-CG-CD1	5.51	120.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	LEU	CB-CG-CD2	5.42	120.21	111.00
1	B	236	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	476	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	202	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3223	0	3127	41	0
1	B	3229	0	3141	31	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	22	0	18	2	0
4	B	22	0	18	1	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	211	0	0	4	0
8	B	175	0	0	3	0
All	All	7031	0	6422	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:CAS:AS	1:A:384:CAS:SG	2.46	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:CAS:AS	1:B:384:CAS:SG	2.59	1.21
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.61	0.83
1:A:108:PRO:HD3	8:A:2029:HOH:O	1.89	0.72
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.08	0.67
1:B:240:ARG:HD2	1:B:241:GLY:O	1.95	0.66
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.27	0.65
1:A:108:PRO:CD	8:A:2029:HOH:O	2.44	0.65
1:A:384:CAS:CB	1:A:384:CAS:AS	3.05	0.64
1:B:384:CAS:SG	1:B:384:CAS:CE1	2.87	0.63
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.65	0.61
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.42	0.60
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.82	0.59
1:A:152:LEU:O	1:A:156:GLU:HG2	2.02	0.59
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.86	0.58
1:A:294:LEU:HD13	1:A:304:LEU:HD12	1.88	0.55
1:B:384:CAS:AS	1:B:384:CAS:CB	3.15	0.55
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.88	0.54
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.38	0.54
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.89	0.53
1:A:240:ARG:HD2	1:A:241:GLY:O	2.08	0.53
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.74	0.53
1:B:323:GLU:CD	1:B:323:GLU:H	2.12	0.53
1:A:240:ARG:CD	1:A:241:GLY:O	2.57	0.52
1:B:427:VAL:HG23	8:B:2145:HOH:O	2.09	0.52
1:B:324:TRP:O	1:B:327:ALA:HB3	2.10	0.52
1:B:378:LEU:HB2	8:B:2134:HOH:O	2.10	0.52
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.93	0.51
2:A:500:HEM:HMC1	2:A:500:HEM:HBC2	1.93	0.51
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.93	0.50
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.94	0.50
1:A:158:GLU:OE2	1:A:166:HIS:HD2	1.95	0.50
1:A:449:TRP:HA	3:A:600:H4B:N1	2.27	0.49
1:A:294:LEU:HD13	1:A:304:LEU:CD1	2.42	0.49
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.43	0.49
1:B:97:THR:HB	1:B:98:PRO:HD2	1.95	0.48
1:A:68:PRO:O	1:B:109:ARG:NH2	2.47	0.48
1:A:338:VAL:HG21	4:A:800:M87:C07	2.45	0.47
1:B:146:GLN:O	1:B:150:GLU:HG3	2.14	0.47
1:B:218:LYS:HD3	1:B:219:TYR:N	2.29	0.47
1:A:392:THR:HB	1:B:423:HIS:HB2	1.97	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HG3	1:B:349:GLU:HB2	1.98	0.46
1:A:149:GLU:O	1:A:153:GLN:HG3	2.16	0.46
1:A:214:CYS:SG	8:A:2083:HOH:O	2.34	0.46
1:A:366:THR:O	1:A:370:CYS:HB2	2.16	0.46
1:A:390:ARG:HB2	1:A:390:ARG:HE	1.63	0.46
1:A:69:LYS:CE	1:A:69:LYS:HA	2.46	0.46
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.98	0.45
1:A:477:TYR:OH	2:A:500:HEM:O2D	2.27	0.45
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.78	0.44
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.98	0.44
8:A:2001:HOH:O	1:B:109:ARG:HG2	2.17	0.44
1:B:384:CAS:AS	1:B:384:CAS:HB2	2.78	0.43
1:A:413:GLN:O	1:A:416:LYS:HE3	2.17	0.43
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.49	0.43
1:A:423:HIS:HB2	1:B:392:THR:HB	2.00	0.43
1:A:105:LEU:HD23	1:A:105:LEU:N	2.34	0.43
1:A:340:ASN:HD22	1:A:340:ASN:H	1.67	0.43
1:B:231:THR:O	1:B:353:ALA:HA	2.19	0.43
1:A:100:ARG:CZ	1:A:102:LEU:HD22	2.49	0.43
1:B:287:ARG:HD3	8:B:2110:HOH:O	2.18	0.43
1:A:363:GLU:OE1	4:A:800:M87:N01	2.52	0.43
1:B:455:SER:CB	1:B:458:LEU:HD22	2.48	0.42
1:A:100:ARG:NH1	1:A:102:LEU:HD22	2.35	0.42
1:A:240:ARG:HD3	1:A:298:PRO:CG	2.50	0.42
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.95	0.42
2:B:500:HEM:HBC2	2:B:500:HEM:HMC1	2.02	0.42
1:A:126:LEU:HD23	1:A:130:ARG:HH21	1.83	0.41
1:A:121:PRO:O	1:A:124:GLN:HB3	2.20	0.41
1:A:240:ARG:HD3	1:A:241:GLY:O	2.20	0.41
1:B:215:ASN:O	1:B:218:LYS:HD3	2.21	0.41
1:B:338:VAL:HG21	4:B:800:M87:C07	2.51	0.40
1:B:472:SER:HA	1:B:473:PRO:C	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/443 (90%)	387 (97%)	13 (3%)	0	100	100
1	B	400/443 (90%)	387 (97%)	12 (3%)	1 (0%)	44	35
All	All	800/886 (90%)	774 (97%)	25 (3%)	1 (0%)	55	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/375 (92%)	325 (95%)	18 (5%)	27	17
1	B	344/375 (92%)	323 (94%)	21 (6%)	22	12
All	All	687/750 (92%)	648 (94%)	39 (6%)	24	14

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	109	ARG
1	A	123	GLU
1	A	125	LEU
1	A	146	GLN
1	A	156	GLU
1	A	226	LEU

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Mol	Chain	Res	Type
1	A	293	LEU
1	A	294	LEU
1	A	298	PRO
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	458	LEU
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	110	LYS
1	B	124	GLN
1	B	143	SER
1	B	207	GLN
1	B	218	LYS
1	B	223	ARG
1	B	225	ASN
1	B	236	ARG
1	B	240	ARG
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	222	ASN
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	CAS	A	384	1	6,8,9	1.59	2 (33%)	2,9,11	0.90	0
1	CAS	B	384	1	6,8,9	1.84	2 (33%)	2,9,11	1.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	A	384	1	-	0/0/7/9	0/0/0/0
1	CAS	B	384	1	-	0/0/7/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE1	2.30	2.02	1.96
1	A	384	CAS	CA-C	2.36	1.53	1.50
1	A	384	CAS	AS-CE2	2.88	2.03	1.96
1	B	384	CAS	AS-CE2	3.19	2.04	1.96



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	3	0
1	B	384	CAS	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	HEM	A	500	1	28,50,50	1.30	5 (17%)	17,82,82	1.80	5 (29%)
3	H4B	A	600	-	14,18,18	1.22	1 (7%)	12,26,26	2.50	4 (33%)
4	M87	A	800	-	24,24,24	1.29	3 (12%)	30,32,32	1.74	7 (23%)
5	ACT	A	860	-	1,3,3	1.59	0	0,3,3	0.00	-
5	ACT	A	861	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
6	GOL	A	880	-	5,5,5	0.84	0	5,5,5	1.39	1 (20%)
2	HEM	B	500	1	28,50,50	1.53	2 (7%)	17,82,82	1.62	4 (23%)
3	H4B	B	600	-	14,18,18	1.26	1 (7%)	12,26,26	2.31	4 (33%)
4	M87	B	800	-	24,24,24	1.27	1 (4%)	30,32,32	1.40	6 (20%)
5	ACT	B	860	-	1,3,3	2.79	1 (100%)	0,3,3	0.00	-
5	ACT	B	861	-	1,3,3	1.03	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.73	0	5,5,5	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1	-	0/6/54/54	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	M87	A	800	-	-	0/7/7/7	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
5	ACT	A	861	-	-	0/0/0/0	0/0/0/0
6	GOL	A	880	-	-	0/4/4/4	0/0/0/0
2	HEM	B	500	1	-	0/6/54/54	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	M87	B	800	-	-	0/7/7/7	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
5	ACT	B	861	-	-	0/0/0/0	0/0/0/0
6	GOL	B	880	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1B-NB	-5.58	1.30	1.36
3	B	600	H4B	C4A-C8A	-3.43	1.34	1.41
2	A	500	HEM	C3B-C2B	-3.32	1.36	1.40
2	B	500	HEM	C3B-C2B	-2.97	1.36	1.40
3	A	600	H4B	C8A-N1	-2.34	1.30	1.34
2	A	500	HEM	C1B-NB	-2.23	1.34	1.36
2	A	500	HEM	CMA-C3A	-2.12	1.47	1.51
2	A	500	HEM	C3D-C2D	-2.12	1.31	1.37
4	A	800	M87	F23-C23	-2.04	1.31	1.36
4	A	800	M87	C24-C23	2.14	1.41	1.37
4	A	800	M87	C10-N01	2.48	1.41	1.37
5	A	861	ACT	CH3-C	2.54	1.52	1.48
5	B	860	ACT	CH3-C	2.79	1.52	1.48
2	A	500	HEM	C4D-ND	3.03	1.40	1.36
4	B	800	M87	C02-N01	4.08	1.37	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	M87	F23-C23-C22	-4.34	111.93	118.24
4	B	800	M87	C11-C08-C09	-3.74	115.90	121.69
4	A	800	M87	C14-C21-C22	-3.63	114.60	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CMA-C3A-C4A	-3.31	123.38	128.46
2	B	500	HEM	CBA-CAA-C2A	-3.24	106.29	112.48
4	A	800	M87	N02-C02-N01	-3.06	116.16	118.06
3	B	600	H4B	N3-C2-N1	-2.75	121.00	125.45
4	B	800	M87	C13-C14-C21	-2.74	107.07	112.81
2	A	500	HEM	CBA-CAA-C2A	-2.72	107.28	112.48
4	A	800	M87	C13-C14-C21	-2.29	108.01	112.81
2	A	500	HEM	CAD-C3D-C2D	-2.22	122.66	129.00
4	B	800	M87	C03-C04-C05	-2.21	117.40	120.83
4	B	800	M87	F23-C23-C22	-2.16	115.10	118.24
4	A	800	M87	C04-C03-C02	-2.10	117.57	119.49
3	A	600	H4B	C4A-C4-N3	-2.03	117.94	123.91
4	B	800	M87	F23-C23-C24	2.03	122.08	118.53
2	B	500	HEM	CAA-CBA-CGA	2.14	116.32	112.66
3	A	600	H4B	C4-N3-C2	2.15	119.15	116.06
2	B	500	HEM	CMC-C2C-C3C	2.26	129.08	124.89
6	A	880	GOL	C3-C2-C1	2.26	120.51	111.52
4	B	800	M87	C09-C10-C05	2.31	121.41	118.95
2	B	500	HEM	CAD-CBD-CGD	2.38	116.73	112.66
4	A	800	M87	C08-C11-N12	2.41	119.09	112.93
2	A	500	HEM	C4A-C3A-C2A	2.48	108.72	107.00
2	A	500	HEM	CAD-CBD-CGD	2.50	116.93	112.66
3	B	600	H4B	N2-C2-N3	2.95	121.95	117.24
3	A	600	H4B	N2-C2-N3	3.16	122.29	117.24
4	A	800	M87	F23-C23-C24	3.54	124.72	118.53
3	B	600	H4B	C2-N1-C8A	3.71	122.88	114.51
3	B	600	H4B	C4-C4A-C8A	5.08	119.16	114.56
3	A	600	H4B	C4-C4A-C8A	6.75	120.68	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	4	0
3	A	600	H4B	1	0
4	A	800	M87	2	0
2	B	500	HEM	3	0
4	B	800	M87	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	404/443 (91%)	-0.15	13 (3%) 48 53	24, 34, 62, 102	0
1	B	404/443 (91%)	-0.25	8 (1%) 65 70	24, 38, 67, 100	0
All	All	808/886 (91%)	-0.20	21 (2%) 56 62	24, 37, 66, 102	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	6.5
1	A	123	GLU	4.1
1	B	261	GLY	4.0
1	A	259	GLN	3.9
1	B	110	LYS	3.1
1	A	160	ALA	3.1
1	A	239	GLY	2.9
1	B	111	LEU	2.8
1	B	260	ASP	2.6
1	A	67	GLY	2.6
1	A	69	LYS	2.5
1	A	146	GLN	2.4
1	A	122	ALA	2.3
1	A	109	ARG	2.3
1	A	450	ILE	2.3
1	B	142	ARG	2.3
1	A	449	TRP	2.2
1	B	223	ARG	2.2
1	A	448	ALA	2.2
1	A	153	GLN	2.1
1	B	263	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CAS	B	384	9/10	0.96	0.08	-	46,48,58,69	0
1	CAS	A	384	9/10	0.97	0.08	-	34,35,61,65	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	B	860	4/4	0.95	0.20	6.69	45,47,50,50	0
5	ACT	B	861	4/4	0.97	0.11	2.44	32,35,37,43	0
6	GOL	B	880	6/6	0.93	0.17	2.11	45,50,57,57	0
4	M87	B	800	22/22	0.95	0.12	0.66	26,31,70,71	0
2	HEM	A	500	43/43	0.98	0.16	0.61	23,26,35,42	0
4	M87	A	800	22/22	0.95	0.15	0.52	23,27,69,74	0
6	GOL	A	880	6/6	0.91	0.13	0.30	43,49,54,56	0
3	H4B	A	600	17/17	0.97	0.15	0.07	25,28,35,35	0
2	HEM	B	500	43/43	0.98	0.10	-0.04	25,28,35,45	0
5	ACT	A	861	4/4	0.98	0.08	-0.17	32,33,35,37	0
3	H4B	B	600	17/17	0.97	0.12	-0.52	23,27,35,39	0
5	ACT	A	860	4/4	0.96	0.12	-0.77	36,45,46,47	0
7	ZN	A	1483	1/1	1.00	0.05	-2.71	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.